



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:22 PM UTC

PDB ID : 6J4Q / pdb_00006j4q
Title : Structural basis of tubulin detyrosination by vasohibins-SVBP enzyme complex and functional implications
Authors : Wang, N.; Bao, H.; Huang, H.
Deposited on : 2019-01-10
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

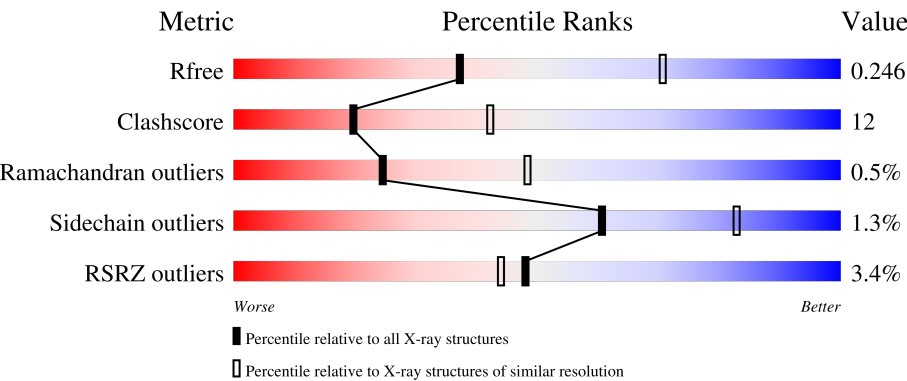
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	251	2% 75% 24% .
1	C	251	2% 76% 20% ..
1	F	251	7% 68% 29% ..
1	J	251	% 82% 16% .
2	B	66	2% 32% 17% 50% .

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Mol	Chain	Length	Quality of chain
2	D	66	5%36%15%48%
2	G	66	2%36%11%52%
2	K	66	5%38%6%56%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9379 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

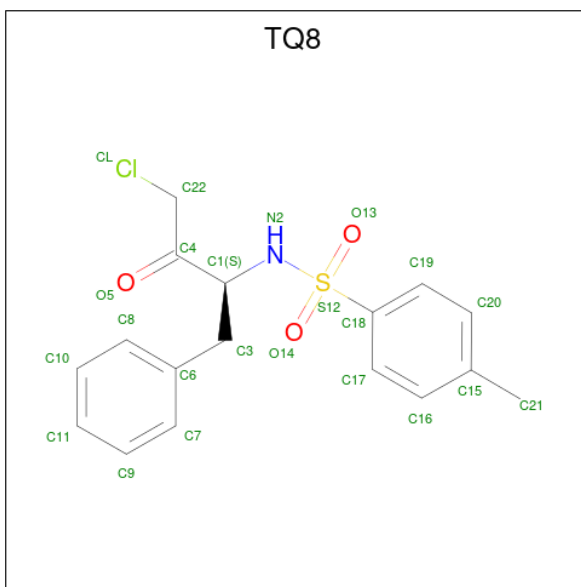
- Molecule 1 is a protein called Tubuliny1-Tyr carboxypeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			2005	1297	348	345	15			
1	C	245	Total	C	N	O	S	0	0	0
			1993	1288	346	345	14			
1	F	246	Total	C	N	O	S	0	0	0
			1990	1285	346	344	15			
1	J	247	Total	C	N	O	S	0	0	0
			1970	1276	336	345	13			

- Molecule 2 is a protein called Small vasohibin-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	33	Total	C	N	O	S	0	0	0
			276	170	51	53	2			
2	D	34	Total	C	N	O	S	0	0	0
			268	163	51	52	2			
2	G	32	Total	C	N	O	S	0	0	0
			239	148	43	46	2			
2	K	29	Total	C	N	O	S	0	0	0
			225	139	42	43	1			

- Molecule 3 is N-[(2S)-4-chloro-3-oxo-1-phenyl-butan-2-yl]-4-methyl-benzenesulfonamide (CCD ID: TQ8) (formula: C₁₇H₁₈ClNO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			22	17	1	3	1		
3	B	1	Total	C	N	O	S	0	0
			22	17	1	3	1		
3	C	1	Total	C	N	O	S	0	0
			22	17	1	3	1		
3	F	1	Total	C	N	O	S	0	0
			22	17	1	3	1		
3	G	1	Total	C	N	O	S	0	0
			22	17	1	3	1		
3	J	1	Total	C	N	O	S	0	0
			22	17	1	3	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		

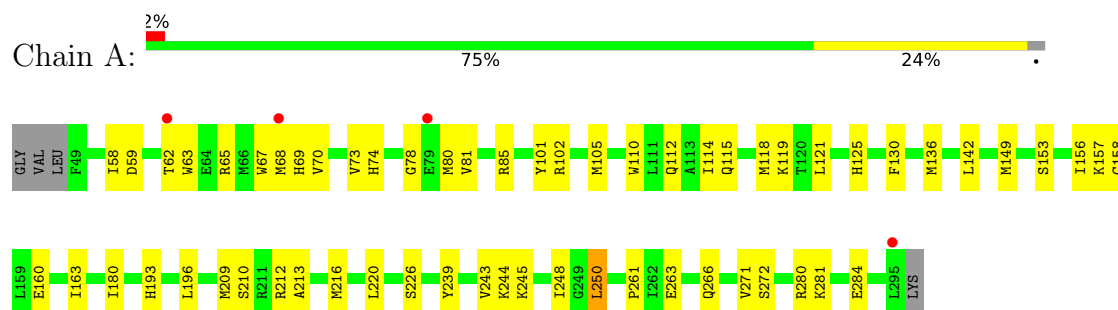
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total	O	0	0
			67	67		
5	B	2	Total	O	0	0
			2	2		
5	C	84	Total	O	0	0
			84	84		
5	D	3	Total	O	0	0
			3	3		
5	F	48	Total	O	0	0
			48	48		
5	G	4	Total	O	0	0
			4	4		
5	J	43	Total	O	0	0
			43	43		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

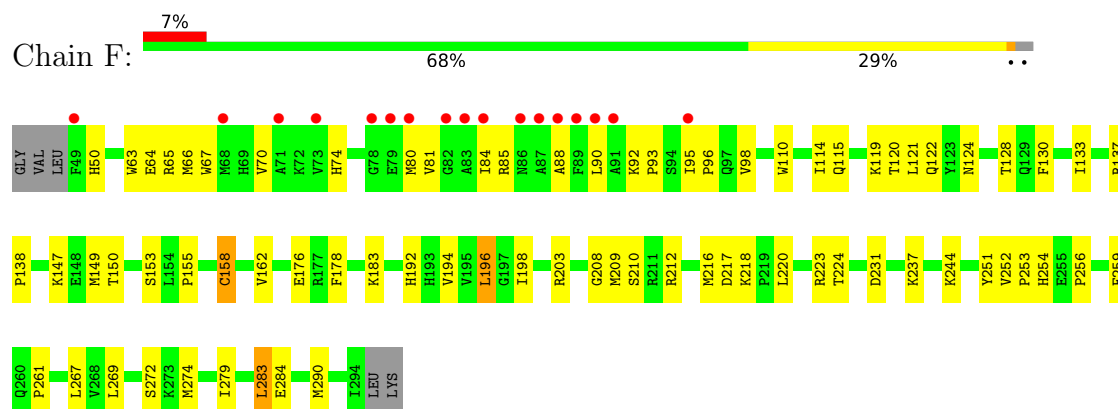
• Molecule 1: Tubuliny-Tyr carboxypeptidase 2



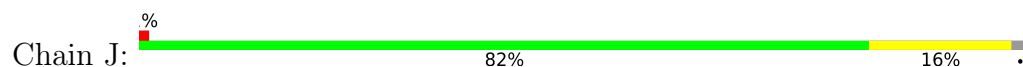
• Molecule 1: Tubuliny-Tyr carboxypeptidase 2

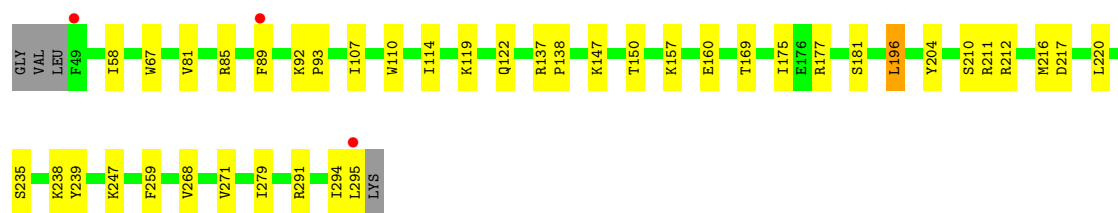


• Molecule 1: Tubuliny-Tyr carboxypeptidase 2

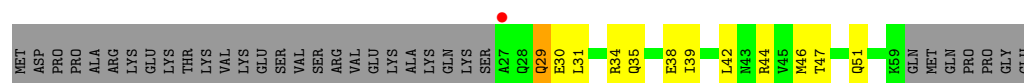
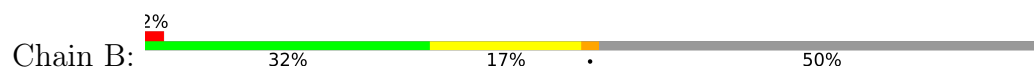


• Molecule 1: Tubuliny-Tyr carboxypeptidase 2

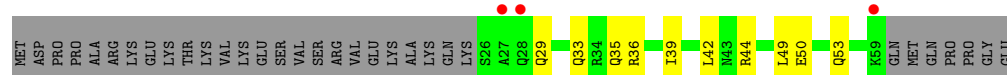
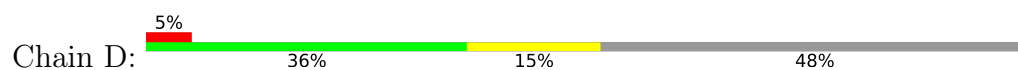




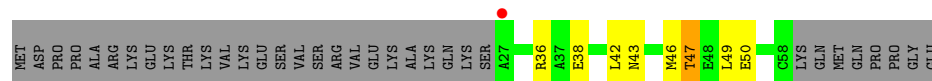
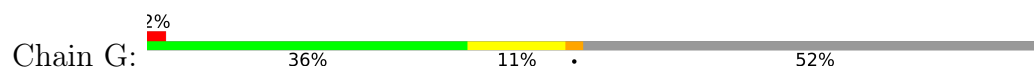
• Molecule 2: Small vasohibin-binding protein



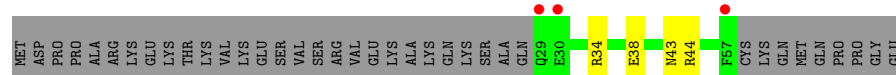
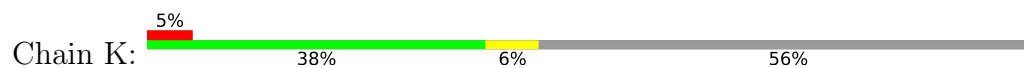
• Molecule 2: Small vasohibin-binding protein



• Molecule 2: Small vasohibin-binding protein



• Molecule 2: Small vasohibin-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.18Å 117.18Å 209.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.31 – 2.70 49.31 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.31-2.70) 93.8 (49.31-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.183 , 0.247 0.183 , 0.246	Depositor DCC
R_{free} test set	2317 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9379	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, TQ8

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	4/2060 (0.2%)	0.71	1/2782 (0.0%)
1	C	0.56	2/2048 (0.1%)	0.71	3/2766 (0.1%)
1	F	0.45	0/2045	0.65	1/2766 (0.0%)
1	J	0.41	0/2025	0.59	0/2744
2	B	0.74	0/278	0.75	0/371
2	D	0.39	0/269	0.56	0/360
2	G	0.61	0/240	0.73	0/323
2	K	0.36	0/226	0.50	0/304
All	All	0.53	6/9191 (0.1%)	0.67	5/12416 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	HIS	C-O	-10.18	1.11	1.23
1	A	281	LYS	C-O	-8.48	1.14	1.24
1	A	281	LYS	N-CA	-6.44	1.38	1.46
1	A	245	LYS	C-O	-6.34	1.16	1.23
1	C	211	ARG	C-O	-5.31	1.17	1.24
1	C	186	PHE	C-O	-5.01	1.17	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	220	LEU	CA-CB-CG	-6.61	93.16	116.30
1	C	121	LEU	CA-C-N	6.42	133.80	121.54
1	C	121	LEU	C-N-CA	6.42	133.80	121.54
1	A	158	CYS	N-CA-C	5.12	116.86	111.28
1	F	158	CYS	CB-CA-C	-5.06	102.88	110.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2005	0	2007	50	0
1	C	1993	0	1991	55	0
1	F	1990	0	1972	57	0
1	J	1970	0	1929	33	0
2	B	276	0	260	9	0
2	D	268	0	249	11	0
2	G	239	0	212	6	0
2	K	225	0	201	3	0
3	A	22	0	16	1	0
3	B	22	0	16	1	0
3	C	22	0	16	1	0
3	F	22	0	16	0	0
3	G	22	0	16	0	0
3	J	22	0	16	1	0
4	A	12	0	16	3	0
4	C	6	0	8	1	0
4	F	6	0	8	0	0
4	J	6	0	8	0	0
5	A	67	0	0	3	0
5	B	2	0	0	1	0
5	C	84	0	0	6	0
5	D	3	0	0	0	0
5	F	48	0	0	5	0
5	G	4	0	0	0	0
5	J	43	0	0	2	0
All	All	9379	0	8957	208	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (208) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:TRP:NE1	5:F:401:HOH:O	1.92	0.92
1:A:101:TYR:HA	1:A:105:MET:HE2	1.55	0.86
1:A:59:ASP:OD1	1:A:62:THR:HG22	1.77	0.85
1:C:151:ARG:NH1	5:C:401:HOH:O	2.06	0.84
1:F:210:SER:HB3	1:F:216:MET:HG2	1.60	0.83
1:F:93:PRO:HB2	2:G:36:ARG:HH12	1.44	0.82
1:J:138:PRO:HB3	1:J:259:PHE:HA	1.64	0.79
1:F:115:GLN:NE2	1:F:208:GLY:O	2.16	0.79
1:J:147:LYS:O	1:J:150:THR:HG22	1.81	0.79
1:A:118:MET:HB2	1:A:209:MET:HE3	1.65	0.78
1:A:213:ALA:HB1	4:A:302:GOL:H12	1.67	0.75
1:F:74:HIS:O	5:F:402:HOH:O	2.05	0.74
1:A:119:LYS:HG2	1:A:209:MET:HE1	1.75	0.69
1:J:169:THR:HB	1:J:175:ILE:HD11	1.73	0.69
1:C:282:GLU:OE2	5:C:402:HOH:O	2.11	0.69
1:A:101:TYR:HA	1:A:105:MET:CE	2.24	0.68
1:F:63:TRP:NE1	5:F:401:HOH:O	2.26	0.68
1:F:50:HIS:CG	1:F:65:ARG:HH11	2.12	0.68
1:A:105:MET:HE1	1:A:110:TRP:CE3	2.29	0.68
1:A:112:GLN:NE2	5:A:401:HOH:O	2.27	0.67
1:J:181:SER:HB2	1:J:247:LYS:HB2	1.76	0.67
1:C:216:MET:HE2	1:C:217:ASP:OD1	1.95	0.66
1:F:115:GLN:OE1	1:F:217:ASP:HB3	1.95	0.66
1:A:58:ILE:HG22	1:A:62:THR:HG23	1.76	0.66
1:A:74:HIS:HD2	1:A:80:MET:HE2	1.60	0.66
1:C:102:ARG:H	1:C:105:MET:CE	2.07	0.66
1:A:149:MET:HE3	1:A:156:ILE:HG21	1.78	0.66
1:C:102:ARG:H	1:C:105:MET:HE3	1.60	0.65
1:C:288:ARG:HA	1:C:291:ARG:HH11	1.61	0.65
1:F:212:ARG:NH1	2:G:50:GLU:OE2	2.28	0.65
1:C:101:TYR:HA	1:C:105:MET:CE	2.27	0.64
2:D:49:LEU:HG	2:D:53:GLN:HE22	1.61	0.64
1:F:237:LYS:NZ	5:F:404:HOH:O	2.26	0.64
1:C:76:LYS:HD3	1:J:89:PHE:HE2	1.63	0.64
1:C:149:MET:HE3	1:C:156:ILE:HG21	1.79	0.64
1:C:110:TRP:NE1	1:C:172:GLN:OE1	2.31	0.63
2:B:44:ARG:NH2	5:B:201:HOH:O	2.32	0.63
1:A:105:MET:HE1	1:A:110:TRP:HE3	1.62	0.63
4:A:302:GOL:H11	1:F:261:PRO:HG3	1.81	0.63
1:A:250:LEU:HD13	1:A:266:GLN:HG3	1.81	0.63
1:F:124:ASN:HB2	1:F:155:PRO:HB2	1.81	0.62
1:A:70:VAL:HG21	2:B:42:LEU:HD21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:HD22	1:A:263:GLU:HG2	1.82	0.62
1:C:212:ARG:HD2	1:C:239:TYR:CE1	2.35	0.61
1:J:211:ARG:HG3	3:J:301:TQ8:O13	2.00	0.61
1:C:143:MET:HE2	1:C:170:ASN:ND2	2.15	0.61
1:C:288:ARG:HA	1:C:291:ARG:NH1	2.15	0.61
1:C:143:MET:HE1	1:C:166:ILE:HG22	1.84	0.60
1:A:74:HIS:CD2	1:A:80:MET:HE2	2.36	0.60
1:C:101:TYR:HA	1:C:105:MET:HE1	1.83	0.60
1:F:274:MET:HE3	1:F:279:ILE:HG12	1.84	0.60
1:F:269:LEU:HB3	1:F:274:MET:HE1	1.82	0.59
1:A:244:LYS:HD2	1:A:272:SER:HB3	1.85	0.59
1:J:81:VAL:O	1:J:85:ARG:HG3	2.03	0.59
1:J:294:ILE:HG22	1:J:295:LEU:HD12	1.86	0.58
1:F:84:ILE:O	5:F:403:HOH:O	2.16	0.58
1:F:74:HIS:HA	2:G:49:LEU:HD11	1.86	0.57
1:J:271:VAL:HG12	1:J:279:ILE:HG12	1.86	0.57
1:C:111:LEU:HD13	1:C:220:LEU:HD13	1.87	0.57
1:A:213:ALA:O	4:A:302:GOL:H31	2.03	0.57
1:F:251:TYR:CD1	1:F:290:MET:HE2	2.40	0.57
1:C:86:ASN:ND2	5:C:408:HOH:O	2.38	0.56
2:D:35:GLN:O	2:D:39:ILE:HG13	2.04	0.56
1:F:269:LEU:HB3	1:F:274:MET:CE	2.36	0.56
1:A:160:GLU:HG3	5:A:443:HOH:O	2.06	0.56
1:C:291:ARG:NH2	5:C:407:HOH:O	2.37	0.56
1:A:102:ARG:H	1:A:105:MET:HE2	1.70	0.55
1:F:95:ILE:HG13	1:F:95:ILE:O	2.06	0.55
1:F:98:VAL:HG21	1:F:150:THR:HG23	1.89	0.55
1:C:102:ARG:NH2	5:C:411:HOH:O	2.40	0.55
1:A:243:VAL:HG12	1:A:271:VAL:HG21	1.89	0.54
2:B:35:GLN:O	2:B:39:ILE:HG13	2.08	0.54
1:C:149:MET:CE	1:C:156:ILE:HG21	2.38	0.54
1:A:250:LEU:CD1	1:A:266:GLN:HG3	2.37	0.54
1:A:250:LEU:HB2	1:A:263:GLU:HB3	1.88	0.53
1:A:81:VAL:O	1:A:85:ARG:HG3	2.08	0.53
1:C:124:ASN:HB3	1:C:157:LYS:HG3	1.90	0.53
1:C:143:MET:CE	1:C:167:TYR:HA	2.38	0.53
1:C:92:LYS:NZ	2:D:36:ARG:HD3	2.23	0.53
1:F:218:LYS:NZ	1:F:231:ASP:OD1	2.34	0.53
1:F:254:HIS:O	1:F:256:PRO:HD3	2.09	0.53
1:C:50:HIS:HB3	1:C:65:ARG:NH1	2.24	0.53
1:F:110:TRP:CE2	1:F:114:ILE:HD11	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:LYS:HD3	1:J:89:PHE:CE2	2.44	0.53
1:J:247:LYS:HG2	1:J:268:VAL:HG13	1.91	0.53
1:C:81:VAL:O	1:C:85:ARG:HG3	2.09	0.52
1:F:66:MET:HG3	1:F:128:THR:HG22	1.92	0.52
1:C:135:LYS:NZ	5:C:413:HOH:O	2.42	0.52
1:A:118:MET:CB	1:A:209:MET:HE3	2.36	0.52
1:F:203:ARG:NH1	1:F:223:ARG:HG2	2.24	0.52
1:F:244:LYS:HA	1:F:272:SER:HB3	1.92	0.52
1:A:69:HIS:O	1:A:73:VAL:HG12	2.10	0.52
1:F:121:LEU:O	1:F:122:GLN:HB2	2.09	0.51
1:A:65:ARG:O	1:A:68:MET:HB3	2.10	0.51
1:C:143:MET:HE1	1:C:167:TYR:HA	1.92	0.51
1:F:85:ARG:HA	2:G:38:GLU:OE2	2.10	0.51
2:K:34:ARG:NE	2:K:38:GLU:OE1	2.42	0.51
1:C:70:VAL:CG1	1:C:80:MET:HE1	2.41	0.51
1:C:111:LEU:CD1	1:C:220:LEU:HD13	2.41	0.51
1:C:149:MET:HE3	1:C:156:ILE:CG2	2.41	0.51
1:F:96:PRO:HB3	1:F:120:THR:HG21	1.93	0.50
1:F:183:LYS:HG3	1:F:192:HIS:CE1	2.46	0.50
1:J:216:MET:HE3	1:J:217:ASP:OD1	2.11	0.50
1:C:70:VAL:HG21	2:D:42:LEU:HD21	1.94	0.50
1:F:124:ASN:ND2	1:F:130:PHE:CE2	2.79	0.50
1:J:122:GLN:HE21	2:K:43:ASN:HD22	1.60	0.50
1:F:224:THR:HB	1:F:284:GLU:OE2	2.11	0.49
1:J:147:LYS:HA	1:J:150:THR:HG22	1.92	0.49
1:C:125:HIS:CD2	2:D:50:GLU:HG2	2.47	0.49
1:A:212:ARG:HD2	1:A:239:TYR:CZ	2.47	0.49
1:A:209:MET:HE2	1:A:216:MET:HE3	1.94	0.49
1:F:251:TYR:CE1	1:F:290:MET:HE2	2.47	0.48
1:J:212:ARG:HD2	1:J:239:TYR:CZ	2.48	0.48
1:F:133:ILE:HD11	1:F:149:MET:HE2	1.96	0.48
1:F:147:LYS:O	1:F:150:THR:HB	2.13	0.48
1:A:62:THR:OG1	1:A:65:ARG:NH2	2.47	0.48
1:A:102:ARG:O	1:A:105:MET:HG3	2.14	0.48
2:B:29:GLN:O	2:B:30:GLU:C	2.55	0.48
1:F:115:GLN:O	1:F:119:LYS:HG3	2.13	0.48
1:A:136:MET:HE3	1:A:261:PRO:HB2	1.95	0.48
1:C:143:MET:HE2	1:C:170:ASN:HD21	1.78	0.48
1:C:50:HIS:HB3	1:C:65:ARG:HH11	1.79	0.47
1:F:216:MET:HB2	1:F:217:ASP:H	1.51	0.47
1:J:204:TYR:OH	1:J:291:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ARG:O	2:B:38:GLU:HG3	2.14	0.47
1:C:92:LYS:HZ2	2:D:36:ARG:HD3	1.78	0.47
1:A:63:TRP:NE1	1:A:67:TRP:HE1	2.12	0.47
1:A:226:SER:OG	1:A:284:GLU:OE2	2.27	0.47
2:D:44:ARG:HD3	2:K:44:ARG:HD3	1.97	0.47
1:J:58:ILE:HD12	1:J:58:ILE:H	1.80	0.47
1:J:110:TRP:CZ2	1:J:114:ILE:HD11	2.50	0.47
1:C:92:LYS:HE3	2:D:36:ARG:HH11	1.80	0.47
1:A:130:PHE:CZ	2:B:39:ILE:HD13	2.50	0.46
2:D:49:LEU:HG	2:D:53:GLN:NE2	2.28	0.46
1:F:90:LEU:HD13	1:F:92:LYS:HB2	1.97	0.46
1:C:56:PHE:HA	1:C:57:PRO:C	2.40	0.46
1:C:212:ARG:HD2	1:C:239:TYR:CZ	2.50	0.46
1:C:280:ARG:O	1:C:284:GLU:HB2	2.15	0.46
1:C:135:LYS:NZ	4:C:302:GOL:H31	2.31	0.45
3:C:301:TQ8:H8	3:C:301:TQ8:H1	1.72	0.45
1:F:198:ILE:HG22	1:F:220:LEU:HD21	1.98	0.45
1:F:279:ILE:HG22	1:F:283:LEU:HD22	1.98	0.45
1:C:121:LEU:O	1:C:122:GLN:HG2	2.15	0.45
1:F:67:TRP:CD1	1:F:85:ARG:HD2	2.51	0.45
1:C:177:ARG:HB3	1:C:196:LEU:HD21	1.99	0.45
1:F:162:VAL:HG21	1:F:194:VAL:HG22	1.99	0.45
1:A:78:GLY:H	1:A:81:VAL:HG23	1.82	0.45
1:A:115:GLN:NE2	1:A:209:MET:CE	2.80	0.45
1:J:138:PRO:HB3	1:J:259:PHE:CA	2.41	0.45
1:A:59:ASP:OD1	1:A:59:ASP:C	2.60	0.45
1:C:90:LEU:HD23	1:C:90:LEU:HA	1.81	0.45
1:J:210:SER:HB3	1:J:216:MET:HG2	1.99	0.45
1:F:138:PRO:HB3	1:F:259:PHE:O	2.16	0.45
1:A:157:LYS:HB2	5:A:443:HOH:O	2.17	0.44
1:A:210:SER:HB3	1:A:216:MET:HG3	2.00	0.44
3:A:301:TQ8:H1	3:A:301:TQ8:H8	1.60	0.44
1:C:217:ASP:C	1:C:218:LYS:HG2	2.42	0.44
1:J:216:MET:HB2	1:J:217:ASP:H	1.52	0.44
1:A:220:LEU:HD12	1:A:220:LEU:HA	1.76	0.44
1:J:137:ARG:HB2	5:J:439:HOH:O	2.18	0.44
1:J:177:ARG:N	1:J:177:ARG:HD3	2.33	0.44
1:A:115:GLN:NE2	1:A:209:MET:HE2	2.33	0.43
1:A:239:TYR:CE1	3:B:101:TQ8:H7	2.53	0.43
1:C:203:ARG:O	1:C:220:LEU:HD23	2.18	0.43
1:C:92:LYS:HE3	2:D:36:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:43:ASN:O	2:G:47:THR:HG23	2.18	0.43
1:J:196:LEU:HD23	1:J:196:LEU:HA	1.88	0.43
1:A:114:ILE:O	1:A:118:MET:HG3	2.19	0.43
1:J:157:LYS:N	1:J:160:GLU:OE2	2.46	0.43
1:J:235:SER:O	1:J:238:LYS:HB2	2.18	0.43
1:C:218:LYS:NZ	1:C:231:ASP:OD1	2.50	0.43
1:A:125:HIS:HB3	2:B:46:MET:HB2	2.01	0.43
1:F:67:TRP:HA	1:F:70:VAL:HB	2.01	0.43
1:F:176:GLU:OE2	1:F:176:GLU:HA	2.19	0.43
2:D:29:GLN:O	2:D:33:GLN:HG3	2.19	0.42
1:F:224:THR:HB	1:F:284:GLU:CD	2.44	0.42
1:A:160:GLU:HG3	1:A:160:GLU:H	1.65	0.42
1:C:136:MET:HE1	1:C:264:TRP:HD1	1.84	0.42
1:F:50:HIS:HB3	1:F:65:ARG:NH1	2.34	0.42
1:F:80:MET:O	1:F:84:ILE:HG13	2.19	0.42
1:J:212:ARG:NH2	5:J:401:HOH:O	2.51	0.42
1:J:107:ILE:O	1:J:110:TRP:HB3	2.19	0.42
1:F:196:LEU:HD23	1:F:196:LEU:HA	1.92	0.42
1:F:252:VAL:HA	1:F:253:PRO:HD2	1.93	0.42
1:C:69:HIS:O	1:C:73:VAL:HG22	2.20	0.42
1:F:137:ARG:HG3	1:F:138:PRO:HD2	2.02	0.42
1:C:68:MET:HE3	1:C:68:MET:HB3	1.79	0.42
1:C:102:ARG:N	1:C:105:MET:CE	2.77	0.42
1:F:70:VAL:HG12	1:F:81:VAL:HG22	2.01	0.42
1:J:220:LEU:HD23	1:J:220:LEU:HA	1.87	0.42
1:A:180:ILE:HG12	1:A:248:ILE:HD13	2.02	0.41
1:C:121:LEU:C	1:C:122:GLN:HG2	2.45	0.41
1:F:64:GLU:CD	1:F:85:ARG:HH12	2.28	0.41
1:A:142:LEU:HD13	1:A:163:ILE:HD12	2.01	0.41
1:F:119:LYS:HA	1:F:209:MET:HE1	2.01	0.41
1:J:147:LYS:C	1:J:150:THR:HG22	2.45	0.41
1:F:244:LYS:HD2	1:F:272:SER:HB3	2.01	0.41
1:A:280:ARG:O	1:A:284:GLU:HB2	2.21	0.41
1:C:71:ALA:HB2	1:C:81:VAL:HG21	2.02	0.41
1:J:92:LYS:HA	1:J:93:PRO:HD3	1.90	0.41
2:B:47:THR:O	2:B:51:GLN:HG3	2.21	0.40
1:F:67:TRP:CZ3	2:G:42:LEU:HD13	2.56	0.40
1:F:178:PHE:CG	1:F:290:MET:HE1	2.57	0.40
1:A:210:SER:N	1:A:216:MET:HG2	2.36	0.40
1:C:216:MET:HE3	1:C:216:MET:HB2	1.98	0.40
1:J:119:LYS:HD2	1:J:216:MET:HE1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:GLN:O	2:B:31:LEU:N	2.54	0.40
1:J:67:TRP:CE3	1:J:81:VAL:HG13	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	245/251 (98%)	234 (96%)	10 (4%)	1 (0%)	30	54
1	C	243/251 (97%)	231 (95%)	11 (4%)	1 (0%)	30	54
1	F	244/251 (97%)	233 (96%)	9 (4%)	2 (1%)	16	37
1	J	245/251 (98%)	232 (95%)	13 (5%)	0	100	100
2	B	31/66 (47%)	29 (94%)	2 (6%)	0	100	100
2	D	32/66 (48%)	31 (97%)	1 (3%)	0	100	100
2	G	30/66 (46%)	28 (93%)	1 (3%)	1 (3%)	3	7
2	K	27/66 (41%)	27 (100%)	0	0	100	100
All	All	1097/1268 (86%)	1045 (95%)	47 (4%)	5 (0%)	24	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	276	ARG
1	F	88	ALA
1	F	153	SER
2	G	47	THR
1	A	153	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/225 (96%)	213 (99%)	3 (1%)	59	82
1	C	215/225 (96%)	213 (99%)	2 (1%)	70	87
1	F	213/225 (95%)	209 (98%)	4 (2%)	50	77
1	J	208/225 (92%)	207 (100%)	1 (0%)	81	92
2	B	28/60 (47%)	27 (96%)	1 (4%)	31	60
2	D	26/60 (43%)	26 (100%)	0	100	100
2	G	21/60 (35%)	20 (95%)	1 (5%)	23	50
2	K	20/60 (33%)	20 (100%)	0	100	100
All	All	947/1140 (83%)	935 (99%)	12 (1%)	61	83

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LEU
1	A	196	LEU
1	A	250	LEU
2	B	29	GLN
1	C	196	LEU
1	C	284	GLU
1	F	158	CYS
1	F	196	LEU
1	F	267	LEU
1	F	283	LEU
2	G	46	MET
1	J	196	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	116	ASN

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Mol	Chain	Res	Type
1	A	189	ASN
1	A	254	HIS
1	C	129	GLN
1	C	241	HIS
2	D	51	GLN
2	D	53	GLN
1	F	122	GLN
1	F	192	HIS
1	F	257	HIS
2	G	35	GLN
1	J	122	GLN
1	J	129	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	J	302	-	5,5,5	1.47	1 (20%)	5,5,5	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	302	-	5,5,5	1.67	2 (40%)	5,5,5	0.82	0
4	GOL	C	302	-	5,5,5	1.24	1 (20%)	5,5,5	0.97	0
3	TQ8	G	101	2	22,23,24	2.19	1 (4%)	28,32,33	2.04	5 (17%)
3	TQ8	C	301	1	22,23,24	2.20	2 (9%)	28,32,33	2.82	5 (17%)
4	GOL	F	302	-	5,5,5	1.35	0	5,5,5	0.80	0
3	TQ8	J	301	1	22,23,24	2.35	1 (4%)	28,32,33	2.75	7 (25%)
4	GOL	A	303	-	5,5,5	1.76	2 (40%)	5,5,5	0.79	0
3	TQ8	F	301	1	22,23,24	2.24	1 (4%)	28,32,33	2.78	5 (17%)
3	TQ8	A	301	1	22,23,24	2.32	2 (9%)	28,32,33	3.52	8 (28%)
3	TQ8	B	101	2	22,23,24	2.49	1 (4%)	28,32,33	1.84	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	J	302	-	-	2/4/4/4	-
4	GOL	A	302	-	-	2/4/4/4	-
4	GOL	C	302	-	-	1/4/4/4	-
3	TQ8	G	101	2	-	2/18/19/21	0/2/2/2
3	TQ8	C	301	1	-	8/18/19/21	0/2/2/2
4	GOL	F	302	-	-	2/4/4/4	-
3	TQ8	J	301	1	-	2/18/19/21	0/2/2/2
4	GOL	A	303	-	-	3/4/4/4	-
3	TQ8	F	301	1	-	4/18/19/21	0/2/2/2
3	TQ8	A	301	1	-	9/18/19/21	0/2/2/2
3	TQ8	B	101	2	-	0/18/19/21	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	101	TQ8	C18-S12	-11.12	1.59	1.76
3	J	301	TQ8	C18-S12	-10.29	1.60	1.76
3	F	301	TQ8	C18-S12	-9.99	1.61	1.76
3	A	301	TQ8	C18-S12	-9.91	1.61	1.76
3	G	101	TQ8	C18-S12	-9.48	1.61	1.76
3	C	301	TQ8	C18-S12	-9.46	1.61	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	GOL	C3-C2	3.06	1.63	1.51
4	A	302	GOL	C1-C2	2.59	1.61	1.51
4	A	302	GOL	C3-C2	2.58	1.61	1.51
3	A	301	TQ8	C1-N2	2.52	1.51	1.46
4	J	302	GOL	C3-C2	2.51	1.61	1.51
4	A	303	GOL	C1-C2	2.26	1.60	1.51
4	C	302	GOL	C3-C2	2.23	1.60	1.51
3	C	301	TQ8	O13-S12	2.20	1.46	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	TQ8	O14-S12-O13	-9.96	107.42	119.52
3	F	301	TQ8	O14-S12-O13	-9.89	107.50	119.52
3	A	301	TQ8	C18-S12-N2	9.58	120.94	107.79
3	A	301	TQ8	C3-C1-N2	9.56	122.25	110.64
3	C	301	TQ8	C3-C1-N2	9.32	121.95	110.64
3	C	301	TQ8	O14-S12-O13	-9.27	108.26	119.52
3	J	301	TQ8	O14-S12-O13	-8.92	108.68	119.52
3	J	301	TQ8	C18-S12-N2	8.87	119.96	107.79
3	F	301	TQ8	C18-S12-N2	8.33	119.22	107.79
3	G	101	TQ8	O14-S12-O13	-8.09	109.69	119.52
3	B	101	TQ8	O14-S12-O13	-7.32	110.64	119.52
3	A	301	TQ8	C19-C18-S12	4.72	124.95	119.76
3	B	101	TQ8	C1-N2-S12	-4.20	112.08	121.30
3	G	101	TQ8	C1-N2-S12	-3.86	112.82	121.30
3	J	301	TQ8	C6-C3-C1	-3.34	104.48	113.36
3	A	301	TQ8	C17-C18-S12	-3.28	116.15	119.76
3	C	301	TQ8	C18-S12-N2	3.23	112.23	107.79
3	J	301	TQ8	C3-C1-N2	-3.20	106.76	110.64
3	C	301	TQ8	O13-S12-N2	3.15	112.59	106.88
3	G	101	TQ8	C18-S12-N2	3.05	111.98	107.79
3	A	301	TQ8	C16-C17-C18	3.02	122.38	119.44
3	C	301	TQ8	C17-C18-S12	2.84	122.88	119.76
3	F	301	TQ8	C19-C18-S12	2.61	122.62	119.76
3	G	101	TQ8	O13-S12-C18	2.54	111.18	107.98
3	F	301	TQ8	C3-C1-N2	-2.41	107.72	110.64
3	A	301	TQ8	C6-C3-C1	-2.31	107.21	113.36
3	J	301	TQ8	O14-S12-N2	2.29	111.04	106.88
3	A	301	TQ8	O14-S12-C18	-2.27	105.11	107.98
3	F	301	TQ8	O14-S12-N2	2.26	110.99	106.88
3	J	301	TQ8	C8-C6-C7	2.16	121.45	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	101	TQ8	C6-C3-C1	2.12	119.01	113.36
3	J	301	TQ8	O13-S12-C18	-2.11	105.31	107.98
3	G	101	TQ8	C3-C1-N2	2.04	113.12	110.64

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	TQ8	C3-C1-N2-S12
3	A	301	TQ8	N2-C1-C4-O5
3	C	301	TQ8	C3-C1-N2-S12
3	F	301	TQ8	C3-C1-C4-O5
3	F	301	TQ8	C3-C1-C4-C22
3	G	101	TQ8	C3-C1-C4-C22
3	J	301	TQ8	C3-C1-C4-C22
4	A	303	GOL	C1-C2-C3-O3
4	A	303	GOL	O2-C2-C3-O3
4	F	302	GOL	C1-C2-C3-O3
4	A	302	GOL	O1-C1-C2-C3
4	J	302	GOL	C1-C2-C3-O3
4	A	302	GOL	O1-C1-C2-O2
4	F	302	GOL	O2-C2-C3-O3
3	A	301	TQ8	C17-C18-S12-O14
3	C	301	TQ8	C19-C18-S12-O14
3	C	301	TQ8	C17-C18-S12-O14
3	A	301	TQ8	C19-C18-S12-O14
4	C	302	GOL	O1-C1-C2-O2
3	C	301	TQ8	C17-C18-S12-N2
3	C	301	TQ8	C19-C18-S12-N2
3	C	301	TQ8	C1-C3-C6-C8
3	A	301	TQ8	C4-C1-N2-S12
4	A	303	GOL	O1-C1-C2-O2
3	C	301	TQ8	C1-C3-C6-C7
3	A	301	TQ8	C1-C3-C6-C8
4	J	302	GOL	O2-C2-C3-O3
3	A	301	TQ8	C1-C3-C6-C7
3	J	301	TQ8	C3-C1-C4-O5
3	C	301	TQ8	N2-C1-C4-O5
3	A	301	TQ8	C17-C18-S12-N2
3	A	301	TQ8	C19-C18-S12-N2
3	F	301	TQ8	C1-C3-C6-C8
3	F	301	TQ8	C1-C3-C6-C7

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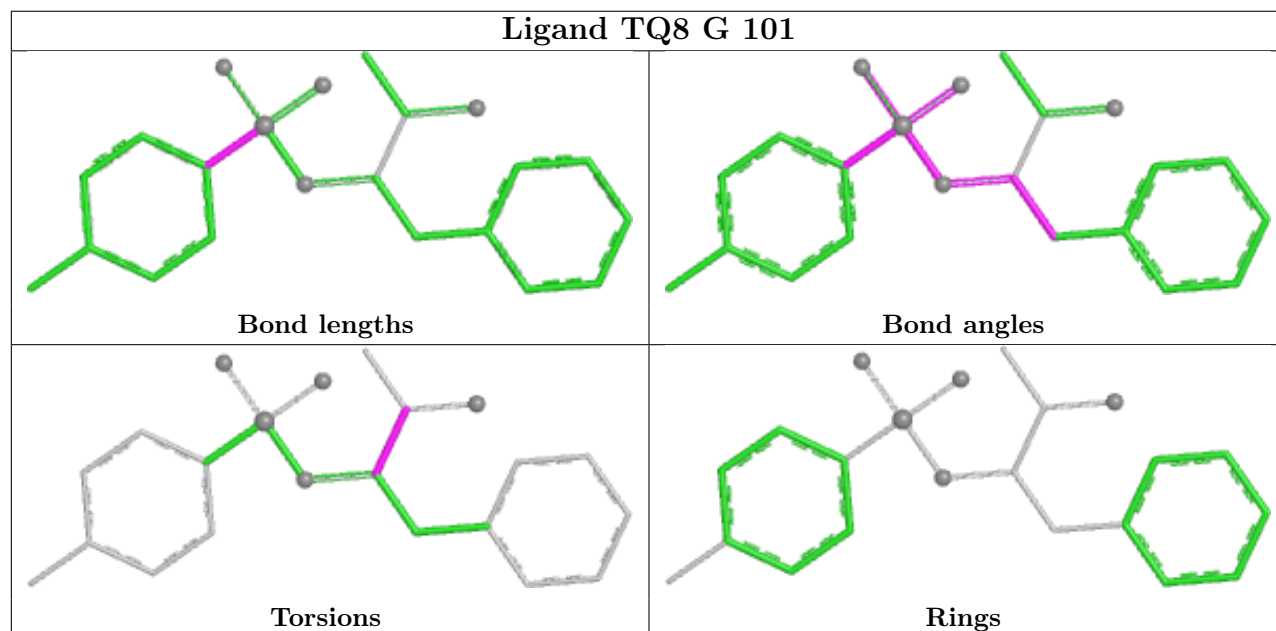
Mol	Chain	Res	Type	Atoms
3	G	101	TQ8	C3-C1-C4-O5

There are no ring outliers.

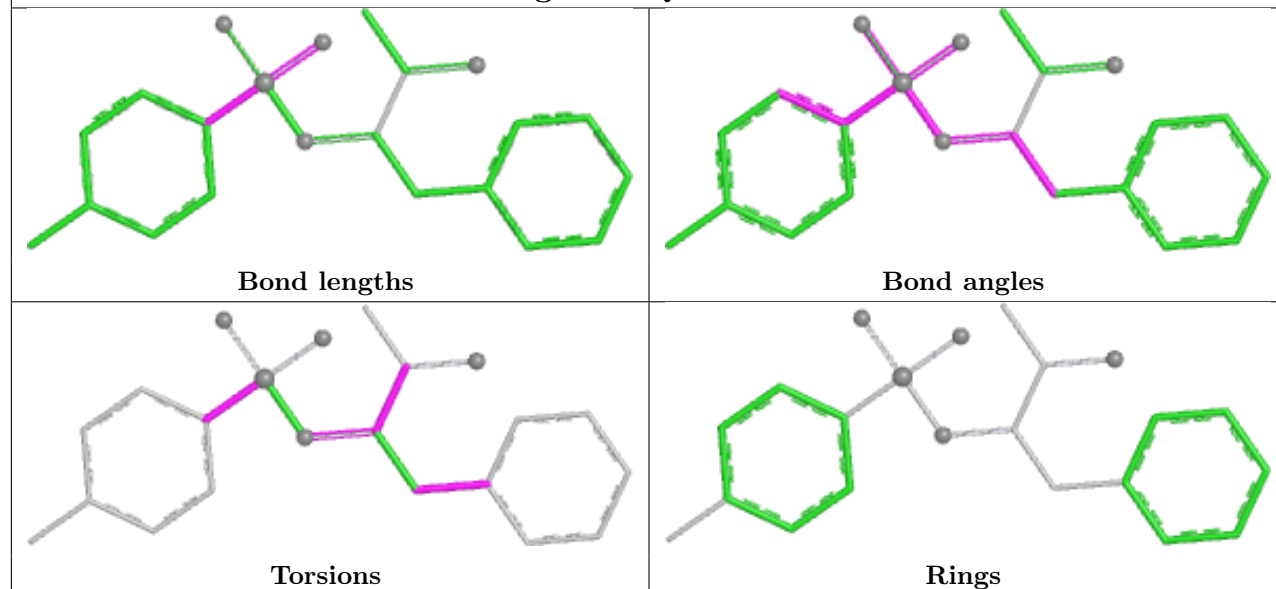
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	GOL	3	0
4	C	302	GOL	1	0
3	C	301	TQ8	1	0
3	J	301	TQ8	1	0
3	A	301	TQ8	1	0
3	B	101	TQ8	1	0

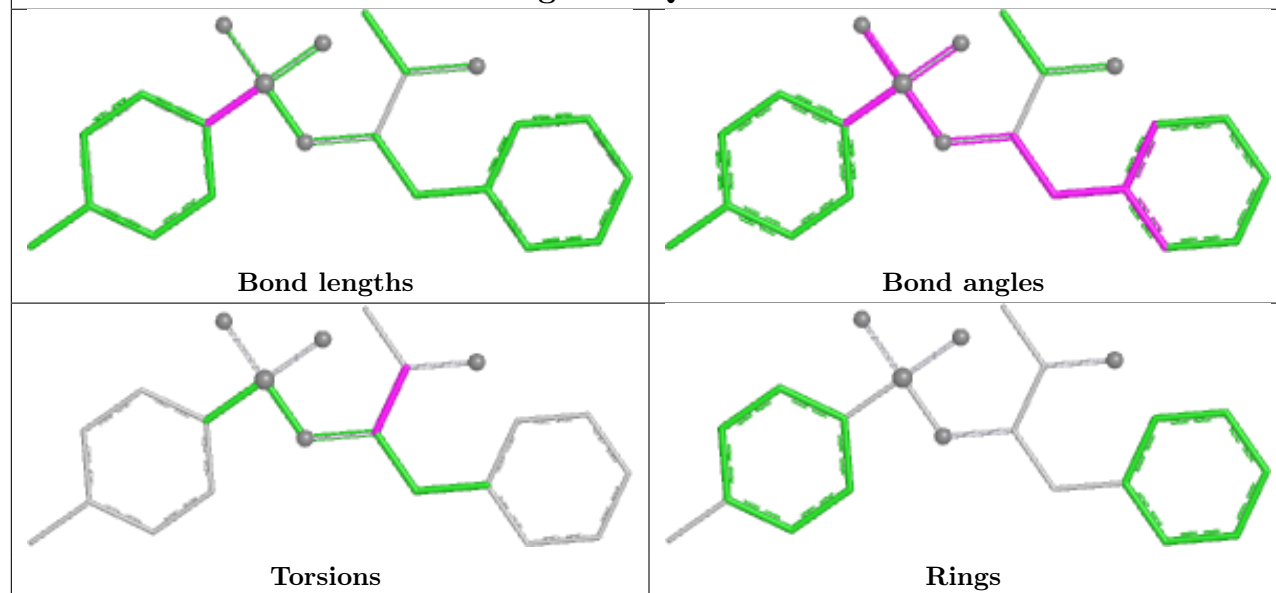
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



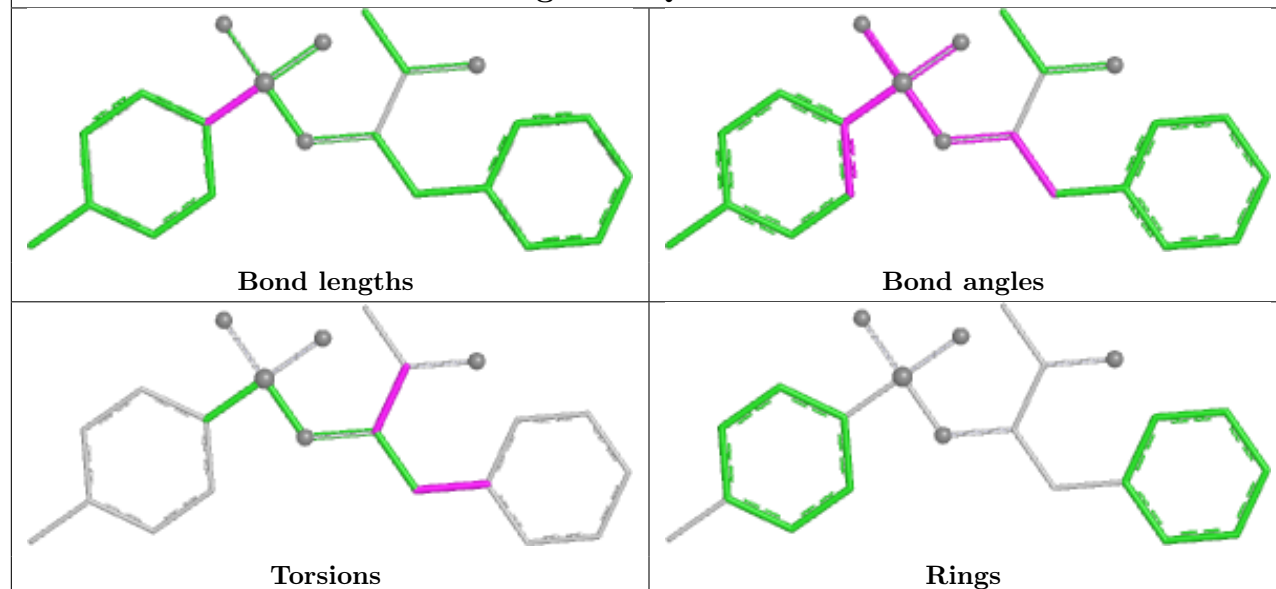
Ligand TQ8 C 301



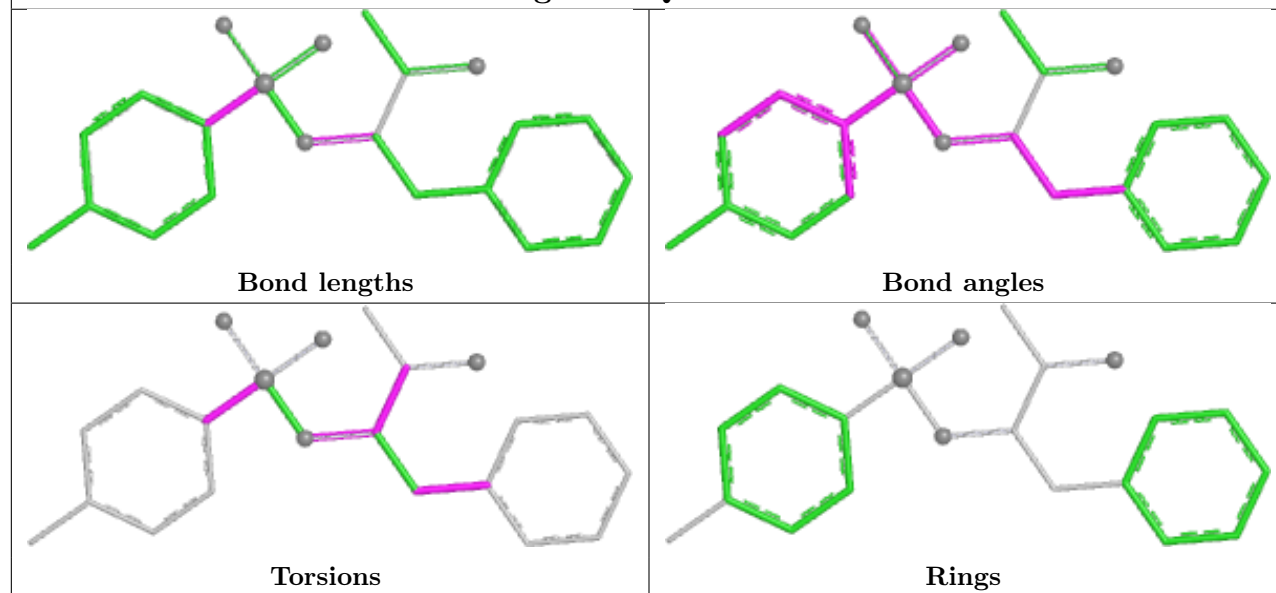
Ligand TQ8 J 301

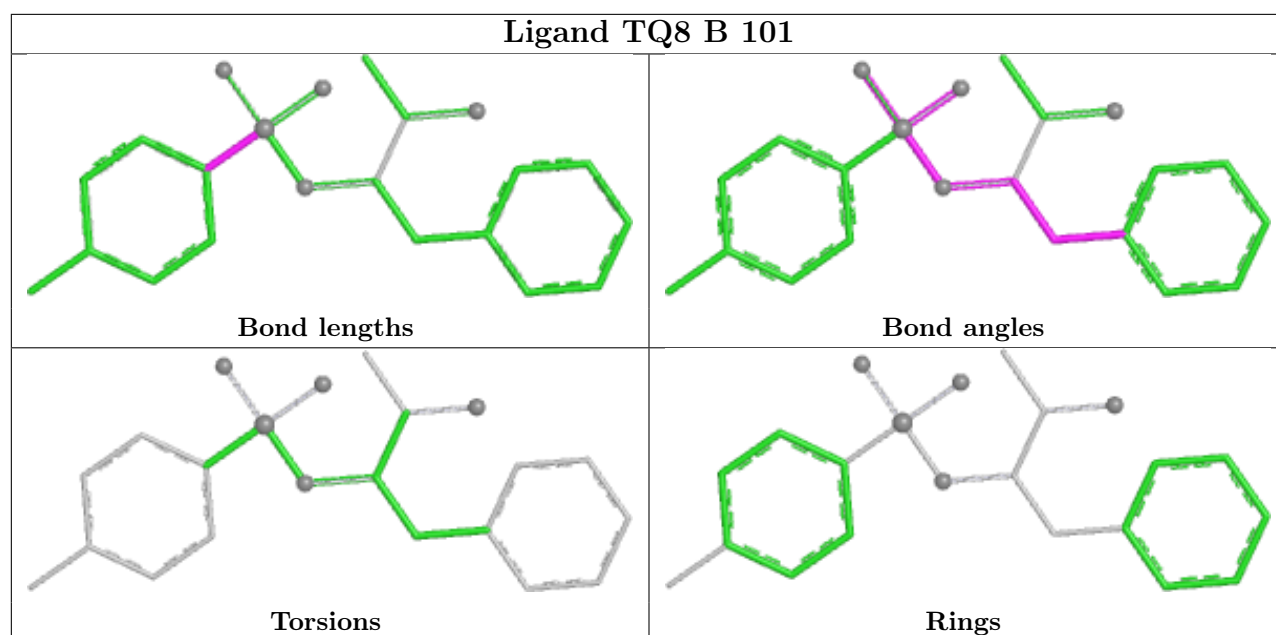


Ligand TQ8 F 301



Ligand TQ8 A 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	247/251 (98%)	-0.30	4 (1%) 70 68	22, 40, 74, 90	0
1	C	245/251 (97%)	-0.37	6 (2%) 59 56	21, 41, 70, 118	0
1	F	246/251 (98%)	-0.02	17 (6%) 23 20	27, 47, 103, 127	0
1	J	247/251 (98%)	-0.18	3 (1%) 76 75	29, 51, 80, 90	0
2	B	33/66 (50%)	0.17	1 (3%) 52 49	36, 57, 97, 102	0
2	D	34/66 (51%)	0.09	3 (8%) 15 13	32, 63, 106, 111	0
2	G	32/66 (48%)	0.83	1 (3%) 51 48	62, 73, 95, 99	0
2	K	29/66 (43%)	0.43	3 (10%) 12 10	44, 62, 89, 96	0
All	All	1113/1268 (87%)	-0.15	38 (3%) 48 44	21, 47, 86, 127	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	91	ALA	6.5
1	F	90	LEU	4.8
1	C	256	PRO	4.4
2	K	57	PHE	4.3
1	F	89	PHE	4.0
1	F	78	GLY	4.0
2	G	27	ALA	3.7
1	F	87	ALA	3.5
2	B	27	ALA	3.4
2	K	29	GLN	3.4
1	C	68	MET	3.3
1	F	80	MET	3.2
1	A	68	MET	3.1
1	J	49	PHE	3.0
1	F	73	VAL	2.9
1	J	295	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	83	ALA	2.7
1	F	71	ALA	2.7
1	F	88	ALA	2.7
1	A	79	GLU	2.6
2	K	30	GLU	2.6
1	C	257	HIS	2.6
2	D	59	LYS	2.5
1	C	259	PHE	2.5
2	D	28	GLN	2.5
1	C	49	PHE	2.4
1	F	84	ILE	2.4
1	F	79	GLU	2.4
2	D	27	ALA	2.4
1	A	62	THR	2.3
1	A	295	LEU	2.2
1	F	95	ILE	2.2
1	F	49	PHE	2.2
1	F	68	MET	2.1
1	F	82	GLY	2.1
1	F	86	ASN	2.1
1	J	89	PHE	2.0
1	C	260	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	J	302	6/6	0.84	0.19	58,77,81,81	0

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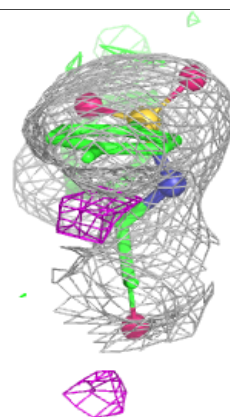
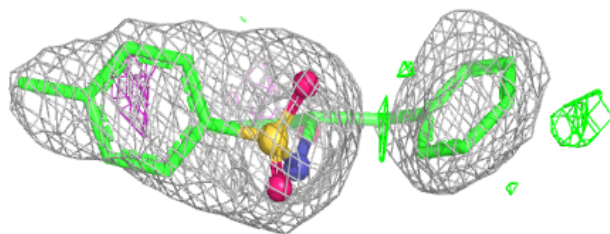
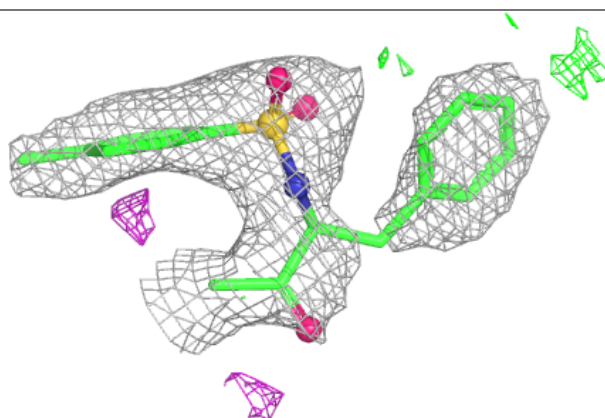
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TQ8	B	101	22/23	0.85	0.16	55,73,88,95	0
4	GOL	F	302	6/6	0.89	0.16	55,59,66,67	0
3	TQ8	G	101	22/23	0.89	0.14	67,75,85,95	0
3	TQ8	F	301	22/23	0.90	0.14	45,66,80,87	0
4	GOL	A	302	6/6	0.91	0.14	44,55,55,56	0
4	GOL	A	303	6/6	0.92	0.15	47,53,55,56	0
4	GOL	C	302	6/6	0.93	0.15	58,61,61,64	0
3	TQ8	J	301	22/23	0.95	0.10	39,57,72,80	0
3	TQ8	A	301	22/23	0.96	0.10	35,50,63,69	0
3	TQ8	C	301	22/23	0.97	0.09	32,52,63,64	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

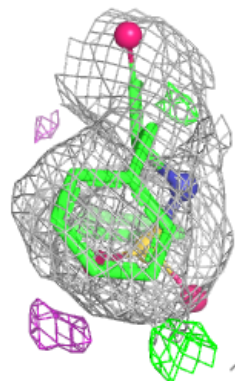
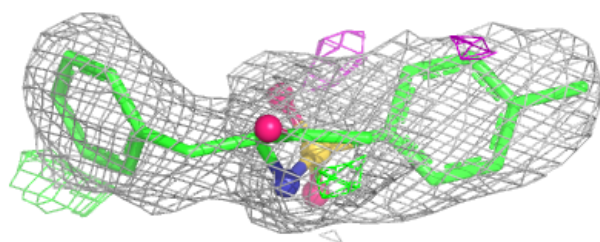
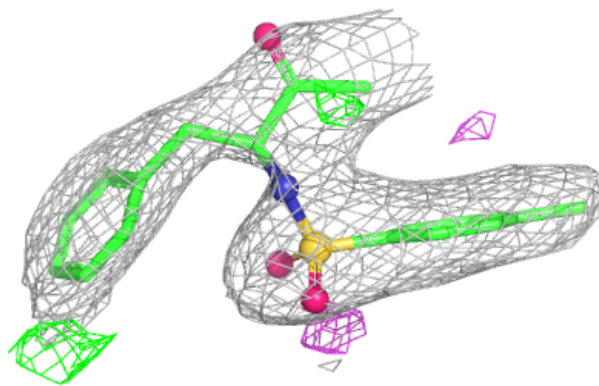
Electron density around TQ8 B 101:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



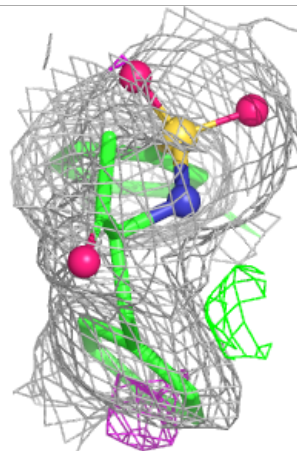
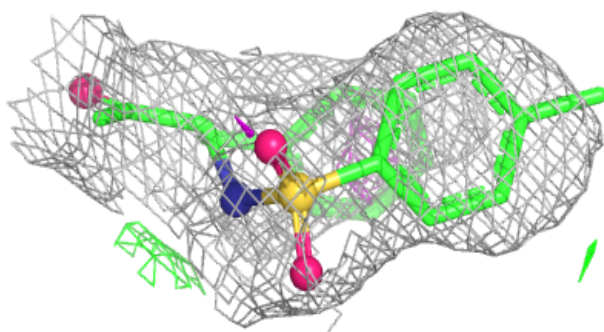
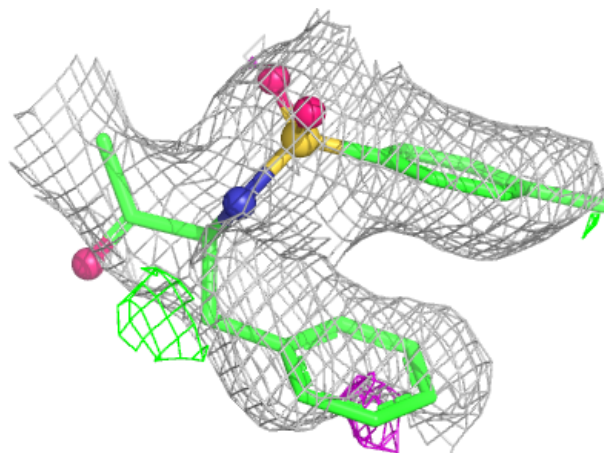
Electron density around TQ8 G 101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



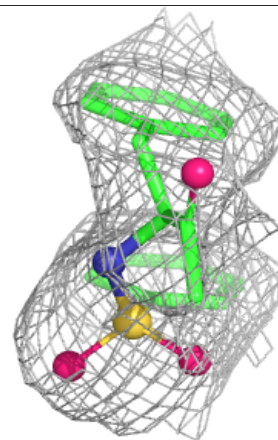
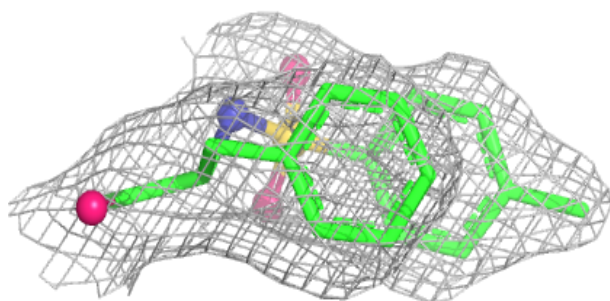
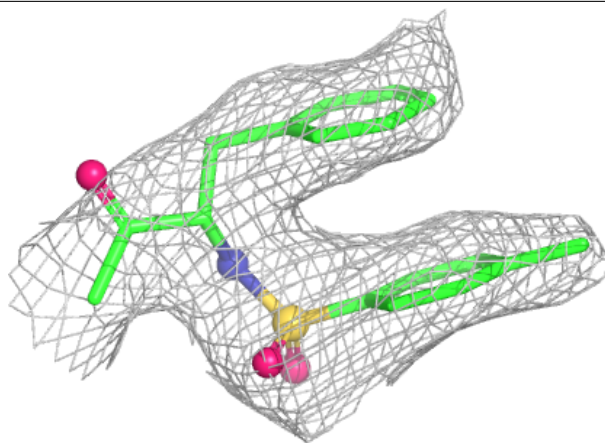
Electron density around TQ8 F 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

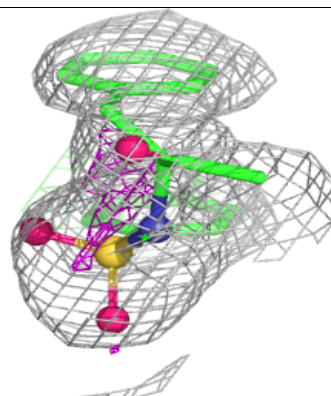
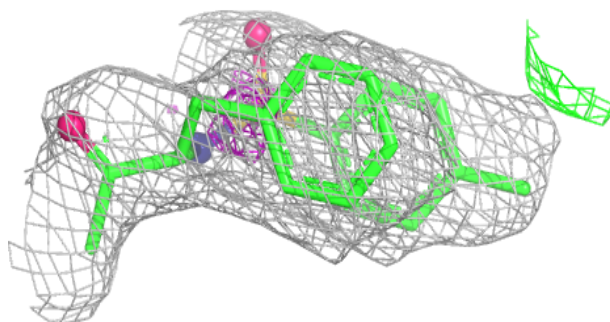
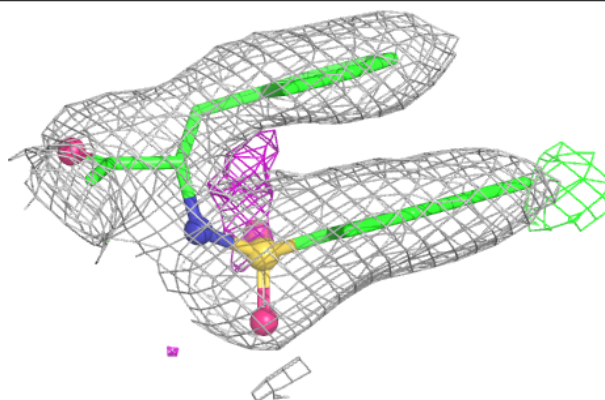


Electron density around TQ8 J 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

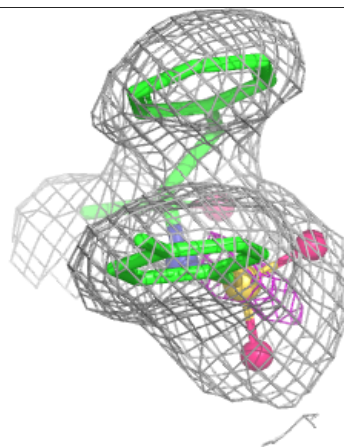
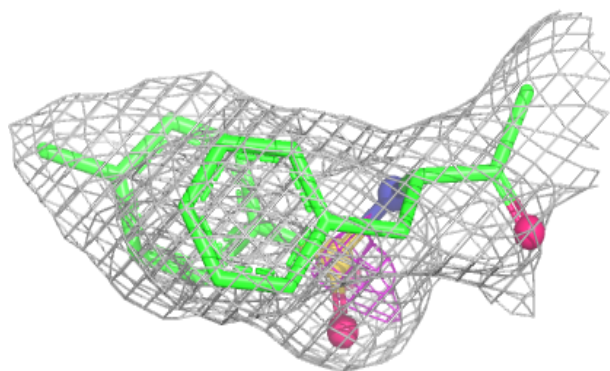
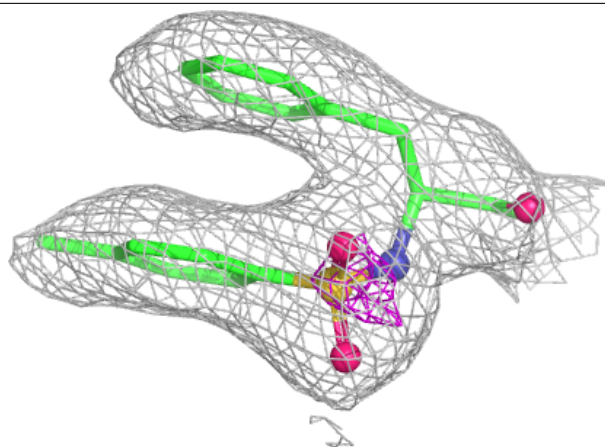
**Electron density around TQ8 A 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TQ8 C 301:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.